

# Signatures of Bose-Einstein condensation in an optical lattice

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We discuss typical experimental signatures for the Bose-Einstein condensation (BEC) of an ultracold Bose gas in an inhomogeneous optical lattice at finite temperature. Applying the Hartree-Fock-Bogoliubov-Popov formalism, we calculate quantities such as the momentum-space density distribution, visibility and peak width as the system is tuned through the superfluid to normal phase transition. Different from previous studies, we consider systems with fixed total particle number, which is of direct experimental relevance. We show that the onset of BEC is accompanied by sharp features in all these signatures, which can be probed via typical time-of-flight imaging techniques. In particular, we find a two-platform structure in the peak width across the phase transition. We show that the onset of condensation is related to the emergence of the higher platform, which can be used as an effective experimental signature.

## I. INTRODUCTION

The realization of Bose-Hubbard model in ultracold atomic gases and the subsequent observation of the superfluid to Mott-insulator phase transition represents a milestone for the quantum simulation of strongly correlated many-body systems in ultracold atomic gases [1–5]. In these experiments, the onset of the superfluid phase is typically connected with the emergence of interference peaks in the time-of-flight images. For example, in Ref. [2], high visibility of interference peaks is taken as an indicator for the existence of superfluidity, while in Ref. [3] and [4], the onset of a bimodal distribution and the rising point of the peak width of the interference pattern in the first Brillouin zone are used as the signature, respectively.

The interference pattern in the post expansion image originates from the existence of short-range correlations. In a uniform non-interacting Bose gas, the short-range correlations can even persist well above the transition temperature, leading to the presence of interference pattern [6]. However, more careful calculations including inter-atomic interactions and global trapping potential confirm a sharp change in visibility at the phase transition point, hence validate the usage of interference pattern as a signature [7–9]. In Ref. [7, 8], it is further suggested that a bimodal structure and the sharp change of the interference peak width in the first Brillouin zone can also serve as an unambiguous signature of superfluidity. In both of these studies, the chemical potentials at the center of the global trapping potential have been fixed, leading to a situation where the total number of particles is not fixed as the temperature is tuned across the ther-

mal phase transition between the superfluid state and the normal state. This scheme is in clear contrast to existing experiments, where the superfluid to normal phase transition is usually tuned through by varying the optical lattice depth with a fixed total particle number [2–4]. To date, a detailed finite-temperature characterization of these experimental signatures for a system with fixed total number of particles is still lacking.

In this work, as an extension to previous studies, we investigate the finite-temperature properties of a trapped ultracold Bose gas throughout the superfluid to normal phase transition, while the total particle number of the system is kept fixed. We apply the Hartree-Fock-Bogoliubov-Popov (HFBP) formalism [10–15], and focus on the characterization of the commonly used signatures of lattice superfluidity, including the visibility, the bimodal structure and the peak width of the interference pattern. We find that all these quantities demonstrate pronounced features as the system crosses the critical point, which can be measured in typical time-of-flight imaging experiments. Interestingly, we demonstrate that as the lattice depth is tuned through the critical depth, a two-platform structure can show up in the peak width measurement of the interference peak in the first Brillouin zone. Based on the results of our calculation, we propose to detect the critical temperature using the second platform as an unambiguous signature.

This paper is organized as the following: in Sec. II, we present the HFBP formalism. In Sec. III, we apply the local density approximation and the HFBP formalism to characterize the momentum distribution of the trapped gas across the critical temperature. We identify sharp features in all three signatures close to the critical temperature for a system with fixed total number of particles. For the peak width in the first Brillouin zone, we propose to associate the critical temperature with the appearance of a second platform. Finally, we summarize in Sec. IV.

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## II. FORMALISM

In this section, we present the HFBP formalism, which, combined with the local density approximation, is used to characterize a trapped BEC at finite temperatures. The Hamiltonian of our system can be written as:

$$H = \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{op}}(\mathbf{r}) + V(\mathbf{r}) \right] \Psi(\mathbf{r}) + \frac{U_{\text{bg}}}{2} \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \Psi(\mathbf{r}). \quad (1)$$

where the lattice potential  $V_{\text{op}}(\mathbf{r}) \equiv V_0 \sum_{i=x,y,z} \sin^2(\pi r_i/d)$  with  $d$  the lattice spacing and  $V_0$  the lattice depth, the global harmonic trapping potential  $V(\mathbf{r}) \equiv m\omega^2 r^2/2$ , and the  $s$ -wave interaction rate  $U_{\text{bg}} = 4\pi\hbar^2 a_s/m$ . We consider the tight-binding case, where the lattice potential is strong enough such that atoms are tightly confined in each lattice site. As a comparison, the global trapping frequency is much weaker. Under these conditions, we can employ the single-band approximation, where the Bose field operators can be expanded in the basis of the Wannier functions  $w(\mathbf{r} - \mathbf{r}_i)$  of the lowest band  $\Psi(\mathbf{r}) = \sum_i w(\mathbf{r} - \mathbf{r}_i) a_i$  [1]. The Hamiltonian Eq. (1) can then be reduced to the Bose-Hubbard Hamiltonian:

$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i - \sum_i \mu_i a_i^\dagger a_i, \quad (2)$$

where the local chemical potential  $\mu_i = \mu(0) - V(\mathbf{r}_i)$  under the local density approximation. In the remainder of this manuscript, we use the recoil energy  $E_R \equiv \hbar^2 \pi^2 / (2md^2)$  as the unit of energy, and the lattice constant  $d$  as the unit of length. In this unit system, the dimensionless hopping rate  $t \approx (3.5/\sqrt{\pi}) s^{3/4} \exp(-2\sqrt{s})$  with  $s \equiv V_0$  [16]. The on-site repulsive interaction rate  $U$  is defined as  $U \equiv U_{\text{bg}} \int |w(\mathbf{r})|^4 d\mathbf{r}$ . In typical experiments, the dimensionless interaction  $U \approx 3.05 s^{0.85} a_s$  [17].

Under the local density approximation, the inhomogeneous Bose gas described by Hamiltonian Eq. (2) can be considered as a group of uniform subsystems with a slowly varying local chemical potential. Each subsystem can then be described by a uniform Hamiltonian, which can be transformed into momentum space by introducing the creation and annihilation operators  $a_{\mathbf{k}}^\dagger$  and  $a_{\mathbf{k}}$ :

$$a_i = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}_i}, \quad a_i^\dagger = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger e^{i\mathbf{k} \cdot \mathbf{r}_i}. \quad (3)$$

Here,  $\mathcal{V}$  is the dimensionless quantization volume, which is the number of lattice sites. Substituting Eq. (3) into

the Bose-Hubbard Hamiltonian Eq. (2), we find:

$$H = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{U}{2\mathcal{V}} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{-\mathbf{k}}^\dagger a_{\mathbf{k}'+\mathbf{q}} a_{-\mathbf{k}'}, \quad (4)$$

where  $\epsilon_{\mathbf{k}} = -2t \sum_{i=x,y,z} \cos(k_i d)$  is the lattice dispersion in the lowest band.

Under the standard HFBP approach, we obtain the effective Hamiltonian [11–13]

$$H_{\text{eff}} \approx (\epsilon_0 - \mu + \frac{U n_0}{2}) N_0 + \sum_{\mathbf{k} \neq 0} [\epsilon_{\mathbf{k}} - \mu + 2U n_{\text{tot}}] a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{U n_0}{2} \sum_{\mathbf{k} \neq 0} [a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}] - \frac{U}{\mathcal{V}} \sum_{\mathbf{k}, \mathbf{k}' \neq 0} n_{\text{ex}}(\mathbf{k}) n_{\text{ex}}(\mathbf{k}'), \quad (5)$$

where  $N_0$  is the total particle number in the condensate with the condensate filling factor  $n_0 = N_0/\mathcal{V}$ , and  $n_{\text{tot}}$  is the total filling factor. Here,  $n_{\text{ex}}(\mathbf{k}) = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle$  for  $\mathbf{k} \neq 0$  is the momentum space distribution of the thermal component, and  $\sum_{\mathbf{k}, \mathbf{k}' \neq 0} n_{\text{ex}}(\mathbf{k}) n_{\text{ex}}(\mathbf{k}') = (N - N_0)^2$ . Under HFBP, the chemical potential is given as:

$$\mu = \left. \frac{dE}{dN} \right|_S = \left. \frac{d\langle H_{\text{eff}} \rangle}{dN} \right|_S. \quad (6)$$

The effective Hamiltonian above can be diagonalized using the standard Bogoliubov transformation:

$$H_{\text{eff}} = (\epsilon_0 - \mu + \frac{U n_0}{2}) N_0 + \frac{1}{2} \sum_{\mathbf{k} \neq 0} [\lambda - (\epsilon_{\mathbf{k}} - \mu + 2U n_{\text{tot}})] + \sum_{\mathbf{k} \neq 0} \lambda \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} - \frac{U}{\mathcal{V}} (N - N_0)^2, \quad (7)$$

where  $\lambda = \sqrt{(\epsilon_{\mathbf{k}} - \mu + 2U n_{\text{tot}})^2 - (U n_0)^2}$  is the quasi-particle dispersion relation and  $\alpha_{\mathbf{k}}^\dagger$  ( $\alpha_{\mathbf{k}}$ ) is the creation (annihilation) operator for the Bogoliubov quasi-particles.

The thermodynamic potential at a finite temperature  $T$  is given by  $\Omega = -(1/\beta) \ln \text{Tr}(e^{-\beta H_{\text{eff}}})$ , where  $\beta = 1/k_B T$  with  $k_B$  the Boltzmann constant. The total filling factor can then be determined by the number equation, leading to

$$n_{\text{tot}} = n_0 + \frac{1}{2\mathcal{V}} \sum_{\mathbf{k} \neq 0} \left[ \frac{\epsilon_{\mathbf{k}} - \epsilon_0 + U n_0}{E_{\mathbf{k}}} \coth \left( \frac{\beta E_{\mathbf{k}}}{2} \right) - 1 \right], \quad (8)$$

where  $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \epsilon_0 + U n_0)^2 - (U n_0)^2}$ . For a normal gas, the number equation can be obtained from Eq. (8)

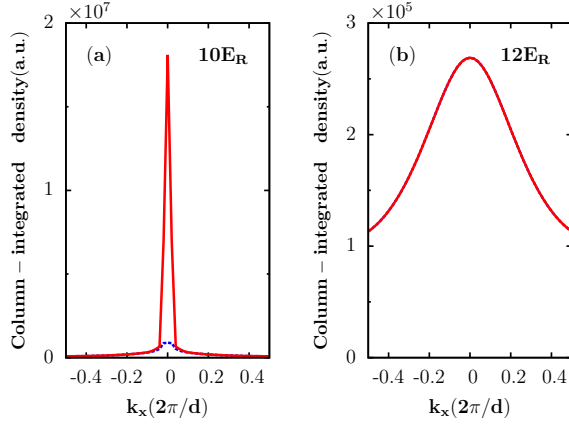


FIG. 1: (Color online) Momentum-space column-integrated density along the  $x$ -axis in the first Brillouin zone. A clear bimodal structure appears when  $V_0$  is below the critical value. Here, the solid curves (red) are the total momentum density distribution, and the dash curves (blue) are the momentum distribution of the thermal component. For the numerical calculations, the trapping frequency  $\omega = 2\pi \times 40$  Hz, the total number  $N = 1.0 \times 10^5$ , and the temperature  $T = 0.18E_R$ . The lattice depth for the subplots are: (a)  $V_0 = 10E_R$ , (b)  $V_0 = 12E_R$ .

by setting  $n_0 = 0$ . The total particle number of such a system is given by

$$N = \int n_{\text{tot}}(\mathbf{r}) d^3\mathbf{r}. \quad (9)$$

We may then solve Eqs. (8) and (9) self-consistently to determine the chemical potential at trap center, the corresponding density and momentum distributions for a given temperature  $T$  and total particle number  $N$ .

### III. EXPERIMENTAL SIGNATURES

In this section, we characterize various experimental signatures for the onset of superfluidity using HFBP formalism, which essentially relies on the calculation of momentum space distribution of the trapped lattice gas. The momentum space distribution can be obtained by transforming the field operator to the momentum space

$$\Psi(\mathbf{k}) = w(\mathbf{k})a_{\mathbf{k}}, \quad (10)$$

where  $\Psi(\mathbf{k})$ ,  $w(\mathbf{k})$  and  $a_{\mathbf{k}}$  are the Fourier components of  $\Psi(\mathbf{r})$ ,  $w(\mathbf{r})$  and  $a_i$ , respectively. As a result, the actual atomic momentum distribution takes the form

$$\begin{aligned} n(\mathbf{k}) &= \langle \Psi^\dagger(\mathbf{k})\Psi(\mathbf{k}) \rangle = |w(\mathbf{k})|^2 \langle a^\dagger(\mathbf{k})a(\mathbf{k}) \rangle \\ &= |w(\mathbf{k})|^2 (n_0(\mathbf{k}) + n_{\text{ex}}(\mathbf{k})), \end{aligned} \quad (11)$$

where  $n_0(\mathbf{k})$  is the momentum space distribution of the condensate. While the momentum distribution of the

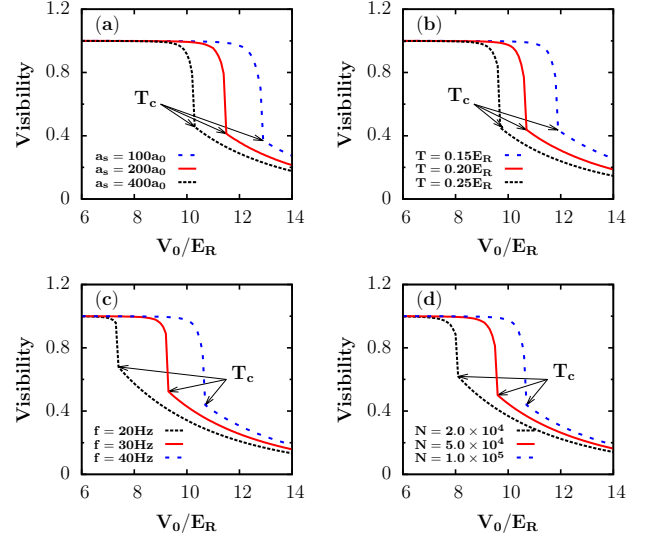


FIG. 2: (Color online) Visibility as a function of scattering length, temperature, trapping frequency and total particle number, respectively. The parameters are: (a)  $T = 0.2E_R$ ,  $\omega = 2\pi \times 40$  Hz and  $N = 1.0 \times 10^5$ ; (b)  $a_s = 320a_0$ ,  $\omega = 2\pi \times 40$  Hz and  $N = 1.0 \times 10^5$ ; (c)  $a_s = 320a_0$ ,  $T = 0.2E_R$  and  $N = 1.0 \times 10^5$ ; (d)  $a_s = 320a_0$ ,  $\omega = 2\pi \times 40$  Hz and  $T = 0.2E_R$ .

thermal gas can be obtained from the trap integration:

$$\begin{aligned} n_{\text{ex}}(\mathbf{k}) &= \\ &= \frac{1}{2V} \int d^3\mathbf{r} \left[ \frac{\epsilon_{\mathbf{k}} - \epsilon_0 + Un_0}{E_{\mathbf{k}}} \coth \frac{\beta E_{\mathbf{k}}}{2} - 1 \right], \end{aligned} \quad (12)$$

the condensate momentum distribution is obtained from the Fourier transformation of the condensate wave function [18]

$$\psi_0(\mathbf{k}) = \frac{1}{\sqrt{V}} \int \psi_0(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r} \quad (13)$$

via the relation  $n_0(\mathbf{k}) = |\psi_0(\mathbf{k})|^2$ .

Experimentally, the momentum distribution of the trapped gas is typically obtained via a time-of-flight image, which is essentially a column-integrated momentum distribution along the direction of the probe laser:

$$n_{\perp}(k_x, k_y) = \int n(\mathbf{k}) dk_z. \quad (14)$$

Here, without loss of generality, we have assumed that the probe laser is applied along the  $z$ -direction. With these, we calculate the column-integrated momentum distribution of the trapped lattice gas at various lattice depths across the critical point, from which we may extract various commonly used signatures for superfluidity.

We first plot in Fig. 1 the column-integrated momentum space density distribution along the  $x$ -axis (with  $k_y = 0$ ) in the first Brillouin zone. Different from the previous studies, we fix the total number  $N = 1.0 \times 10^5$

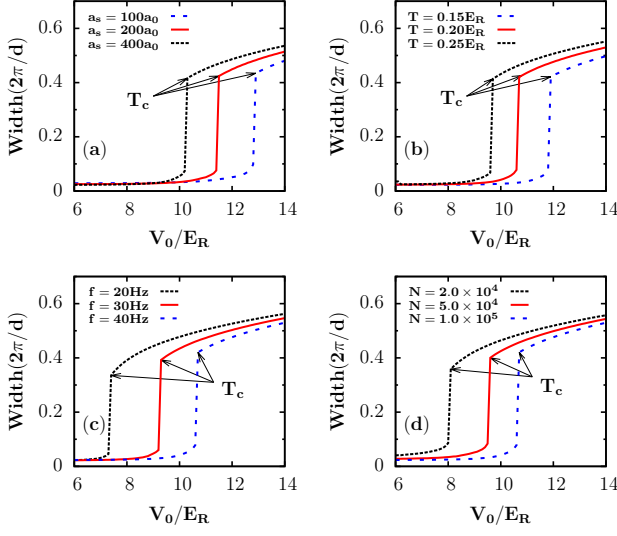


FIG. 3: (Color online) Peak width as a function of scattering length, temperature, trapping frequency and total particle number, respectively. The parameters are: (a)  $T = 0.2E_R$ ,  $\omega = 2\pi \times 40$  Hz and  $N = 1.0 \times 10^5$ ; (b)  $a_s = 320a_0$ ,  $\omega = 2\pi \times 40$  Hz and  $N = 1.0 \times 10^5$ ; (c)  $a_s = 320a_0$ ,  $T = 0.2E_R$  and  $N = 1.0 \times 10^5$ ; (d)  $a_s = 320a_0$ ,  $\omega = 2\pi \times 40$  Hz and  $T = 0.2E_R$ .

at a given temperature  $T = 0.18E_R$ . The parameters are chosen in close relation to existing experiments [4]. From Fig. 1, we see that bimodal structures emerge as soon as the optical lattice depth is below the critical point. This is qualitatively consistent with the results in Ref. [7, 8], where the total particle number is not fixed.

Another commonly used signature for the onset of superfluidity is the visibility of the interference pattern [17]

$$v = \frac{n_{\perp}^A - n_{\perp}^B}{n_{\perp}^A + n_{\perp}^B}, \quad (15)$$

where  $n_{\perp}^A$  and  $n_{\perp}^B$  are column-integrated atomic intensities at site  $A$  and  $B$ , respectively. Here, point  $A$  represents the position of a secondary peak while point  $B$  is along a diagonal with the same distance to the central peak as point  $A$ . Fig. 2 shows the visibility as a function of the scattering length, temperature, trapping frequency and the total particle number. We find that the visibility monotonically decreases from unity to a finite value by increasing the lattice depth. The finite visibility at temperatures above  $T_c$  originates from the short-range correlations which are also present in a normal gas. However, we notice that the visibility undergoes a sharp transition by crossing the critical optical lattice depth, indicating its validity as a superfluid transition signature. We also observe that the value of this residual visibility closely depends on the global harmonic trap and the total particle number, as shown in Fig. 2(c) and 2(d).

In order to characterize the sharpness of the atomic momentum distribution in the first Brillouin zone, an-

other commonly used single-value parameter is the peak width of the interference pattern, which is defined as the half-peak width of  $n_{\perp}(k_x, k_y)$  within the first Brillouin zone along  $k_y = 0$

$$n_{\text{mid}} \equiv \frac{1}{2} [n_{k_x}^{\text{max}} + n_{k_x}^{\text{min}}]. \quad (16)$$

In Fig.3 we show the peak width as a function of scattering length, temperature, trapping frequency and the total particle number. Notice that the peak width increases monotonically with the lattice depth, and undergoes a sharp change by crossing the critical transition point. Interestingly, the peak width around the critical point typically features a two-platform structure, where we find that the second platform at a higher lattice depth is associated with the superfluid to normal phase transition. Indeed, the peak width features a sharp increase with an upward curvature when the system is still in the superfluid region, and saturates when crossing the critical point. Thus, we suggest that it is the second platform with saturating peak width that should be used as an unambiguous signal for the phase transition, while the rising point which are used in existing experiments is still within the superfluid region [4]. Besides, we also notice that the saturating value of peak width is also closely related to the global trapping potential and total particle number.

#### IV. CONCLUSION

In summary, we have studied the finite-temperature properties of a trapped ultracold Bose gas throughout the superfluid to normal phase transition, where the number of total particles is fixed. Applying the HFBP formalism, we characterize various signatures associated with the column-integrated momentum distribution of the lattice gas, which can be probed using typical time-of-flight imaging techniques. From our calculations, we find that across the critical point, sharp features can be identified in all signatures we considered, including the visibility and the peak width of the interference pattern. In particular, we identify a two-platform structure in the width of the interference peak in the first Brillouin zone as the lattice depth is tuned. We show that it is the higher platform in this two-platform structure that should be used as a signature for the superfluid to normal phase transition.

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